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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	OCT 04	Precision of EMBASE searching enhanced with new chemical name field
NEWS	3	OCT 06	Increase your retrieval consistency with new formats or for Taiwanese application numbers in CA/CAPLUS.
NEWS	4	OCT 21	CA/CAPLUS kind code changes for Chinese patents increase consistency, save time
NEWS	5	OCT 22	New version of STN Viewer preserves custom highlighting of terms when patent documents are saved in .rtf format
NEWS	6	OCT 28	INPADOCDB/INPAFAMDB: Enhancements to the US national patent classification.
NEWS	7	NOV 03	New format for Korean patent application numbers in CA/CAPLUS increases consistency, saves time.
NEWS	8	NOV 04	Selected STN databases scheduled for removal on December 31, 2010
NEWS	9	NOV 18	PROUSDDR and SYNTHLINE Scheduled for Removal December 31, 2010 by Request of Prous Science
NEWS	10	NOV 22	Higher System Limits Increase the Power of STN Substance-Based Searching
NEWS	11	NOV 24	Search an additional 46,850 records with MEDLINE backfile extension to 1946
NEWS	12	DEC 14	New PNK Field Allows More Precise Crossover among STN Patent Databases
NEWS	13	DEC 18	ReaxysFile available on STN
NEWS	14	DEC 21	CAS Learning Solutions -- a new online training experience
NEWS	15	DEC 22	Value-Added Indexing Improves Access to World Traditional Medicine Patents in CAPLUS
NEWS	16	JAN 24	The new and enhanced DPCI file on STN has been released
NEWS	17	JAN 26	Improved Timeliness of CAS Indexing Adds Value to USPATFULL and USPAT2 Chemistry Patents
NEWS	18	JAN 26	Updated MeSH vocabulary, new structured abstracts, and other enhancements improve searching in STN reload of MEDLINE

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:07:03 ON 26 JAN 2011

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.23

0.23

FILE 'REGISTRY' ENTERED AT 17:07:21 ON 26 JAN 2011

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STRUCTURE FILE UPDATES: 25 JAN 2011 HIGHEST RN 1260485-87-7

DICTIONARY FILE UPDATES: 25 JAN 2011 HIGHEST RN 1260485-87-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

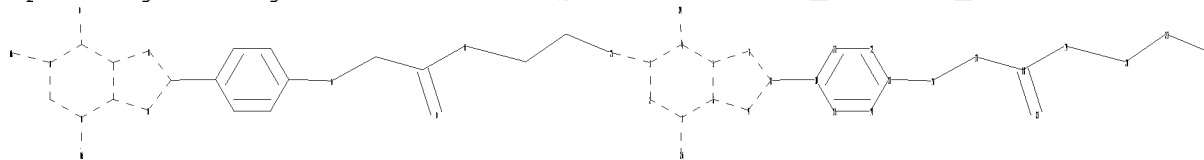
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10551475_01262011_1.str



chain nodes :

16 17 18 19 20 21 22 23 24 25 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

1-26 3-25 4-24 8-10 13-16 16-17 17-18 18-19 18-23 19-20 20-21 21-22

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
 14-15
 exact/norm bonds :
 1-2 1-6 1-26 2-3 3-4 3-25 4-5 4-24 5-6 5-7 6-9 7-8 8-9 13-16 16-17
 18-19 18-23 19-20 21-22
 exact bonds :
 8-10 17-18 20-21
 normalized bonds :
 10-11 10-15 11-12 12-13 13-14 14-15

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam

SAMPLE SEARCH INITIATED 17:07:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS

13 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 93 TO 587

PROJECTED ANSWERS: 44 TO 476

L2 13 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:07:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 335 TO ITERATE

100.0% PROCESSED 335 ITERATIONS

284 ANSWERS

SEARCH TIME: 00.00.01

L3 284 SEA SSS FUL L1

=> s l3 and caplus/lc

73508160 CAPLUS/LC

L4 254 L3 AND CAPLUS/LC

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

202.56

202.79

FILE 'CAPLUS' ENTERED AT 17:07:56 ON 26 JAN 2011
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 26 Jan 2011 VOL 154 ISS 5
FILE LAST UPDATED: 25 Jan 2011 (20110125/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2010

Caplus now includes complete International Patent Classification (IPC) reclassification data for the fourth quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14

L5 166 L4

=> s 15 and fluores?

624698 FLUORES?

L6 8 L5 AND FLUORES?

=> d 16 ibib gi abs hitstr 1-8

L6 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2010:319211 CAPLUS

DOCUMENT NUMBER: 152:542077

TITLE: Influence of fluorophore and linker composition on the pharmacology of fluorescent adenosine A1 receptor ligands

AUTHOR(S): Baker, Jillian G.; Middleton, Richard; Adams, Luke; May, Lauren T.; Briddon, Stephen J.; Kellam, Barrie; Hill, Stephen J.

CORPORATE SOURCE: Institute of Cell Signalling, School of Biomedical Sciences, Medical School, Queen's Medical Centre, University of Nottingham, Nottingham, UK

SOURCE: British Journal of Pharmacology (2010), 159(4), 772-786
CODEN: BJPCBM; ISSN: 1476-5381
URL: <http://www3.interscience.wiley.com/journal/123262>
580/abstract

PUBLISHER: Wiley-Blackwell

DOCUMENT TYPE: Journal; (online computer file)

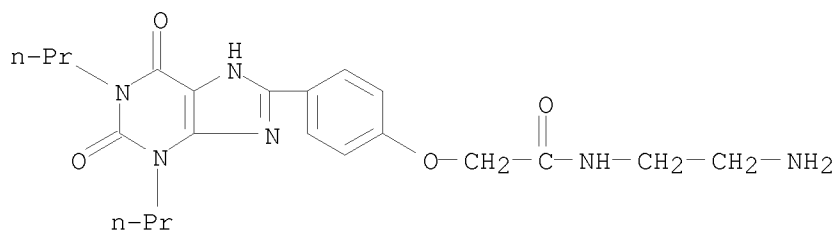
LANGUAGE: English

OTHER SOURCE(S): CASREACT 152:542077

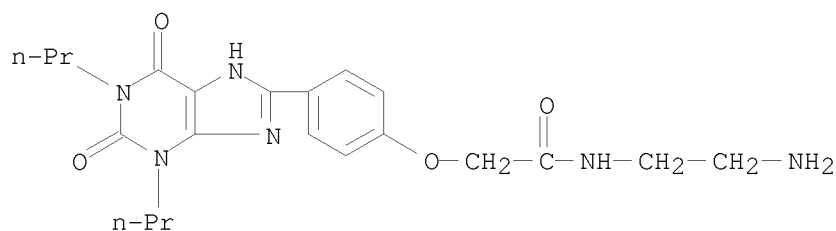
AB Background and purpose: The introduction of fluorescence-based

techniques, and in particular the development of fluorescent ligands, has allowed the study of G protein-coupled receptor pharmacol. at the single cell and single mol. level. This study evaluated how the physicochem. nature of the linker and the fluorophore affected the pharmacol. properties of fluorescent agonists and antagonists. Exptl. approach: Chinese hamster ovary cells stably expressing the human adenosine A1 receptor and a cyclic 3',5' adenosine monophosphate response element-secreted placental alkaline phosphatase (CRE-SPAP) reporter gene, together with whole cell [3H]-8-cyclopentyl-1,3-dipropylxanthine (DPCPX) radioligand binding, were used to evaluate the pharmacol. properties of a range of fluorescent ligands based on the antagonist xanthine amine congener (XAC) and the agonist 5' (N-ethylcarboxamido) adenosine (NECA). Key results: Derivs. of NECA and XAC with different fluorophores, but equivalent linker length, showed significant differences in their binding properties to the adenosine A1 receptor. The BODIPY 630/650 derivs. had the highest affinity. Linker length also affected the pharmacol. properties, depending on the fluorophore used. Particularly in fluorescent agonists, higher agonist potency could be achieved with large or small linkers for dansyl and BODIPY 630/650 derivs., resp. Conclusions and implications: The pharmacol. of a fluorescent ligand was critically influenced by both the fluorophore and the associated linker. Furthermore, the authors' data strongly suggest that the physicochem. properties of the fluorophore/linker pairing determine where in the environment of the target receptor the fluorophore is placed, and this, together with the environmental sensitivity of the resulting fluorescence, may finally decide its utility as a fluorescent probe.

IT 96865-92-8, XAC
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (influence of fluorophore and linker composition on pharmacol. of
 fluorescent adenosine A1 receptor ligands)
 RN 96865-92-8 CAPLUS
 CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-
 dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



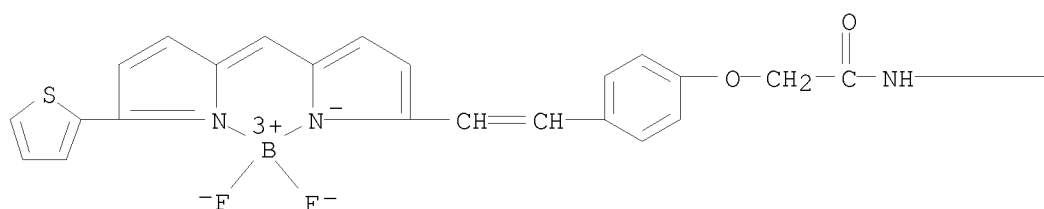
IT 96865-92-8DP, XAC, derivs. 690267-56-2P
 1224605-11-1P 1224605-12-2P 1224605-13-3P
 1224605-14-4P 1224605-15-5P 1224605-16-6P
 1224699-44-8P
 RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (influence of fluorophore and linker composition on pharmacol. of
 fluorescent adenosine A1 receptor ligands)
 RN 96865-92-8 CAPLUS
 CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-
 dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



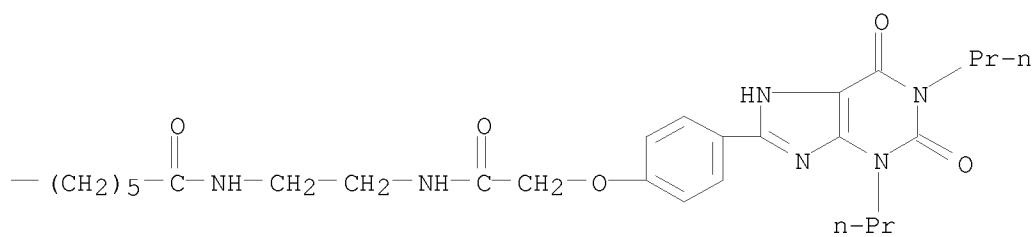
RN 690267-56-2 CAPLUS

CN Boron, difluoro[N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-6-[[[4-[(1E)-2-[5-[5-(2-thienyl)-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-2-yl-κN]ethenyl]phenoxy]acetyl]amino]hexanamidato]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



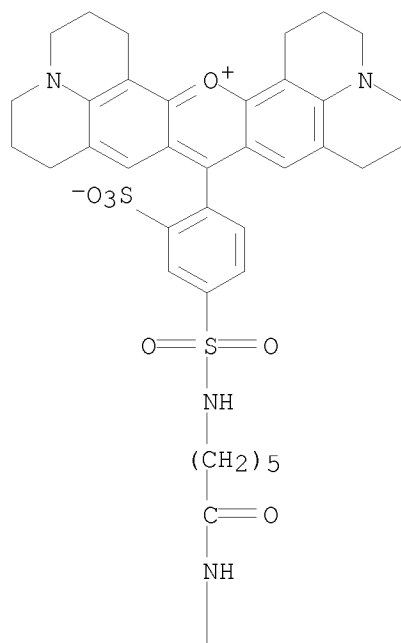
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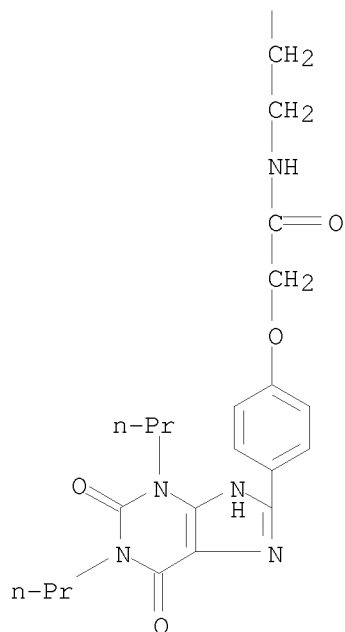
RN 1224605-11-1 CAPLUS

CN 1H,5H,11H,15H-Xantheno[2,3,4-ij:5,6,7-i'j']diquinolizin-18-ium, 2,3,6,7,12,13,16,17-octahydro-9-[4-[[[6-oxo-6-[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]hexyl]amino]sulfonyl]-2-sulfohenyl]-, inner salt (CA INDEX NAME)

PAGE 1-A

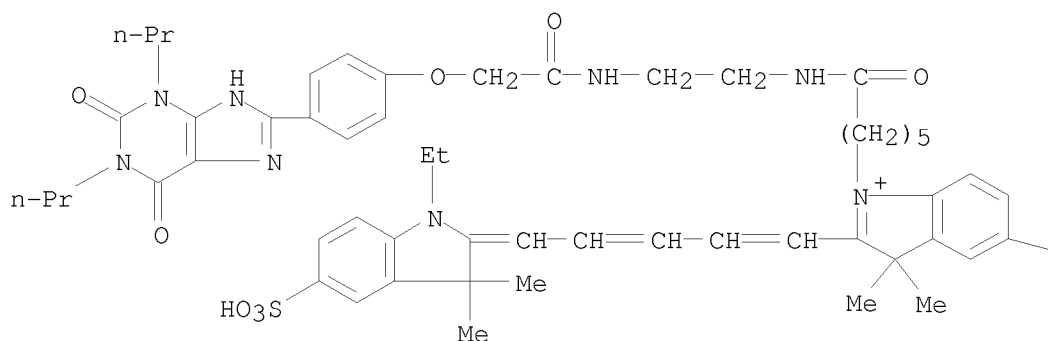


PAGE 2-A



RN 1224605-12-2 CAPLUS
 CN 3H-Indolium, 2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadien-1-yl]-3,3-dimethyl-1-[6-oxo-6-[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]hexyl]-5-sulfo-, inner salt (CA INDEX NAME)

PAGE 1-A

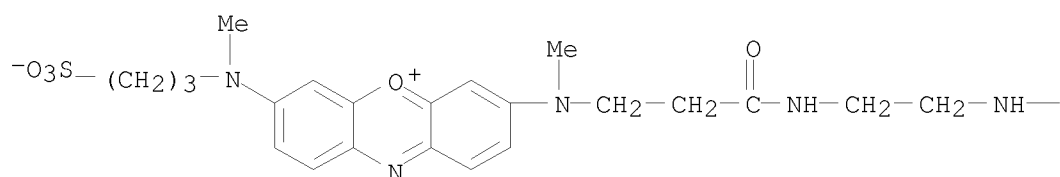


PAGE 1-B

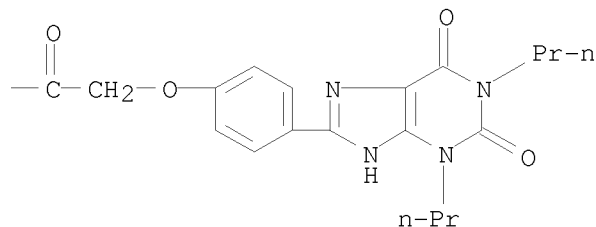


RN 1224605-13-3 CAPLUS
 CN Phenoxazin-5-ium, 3-[methyl[3-oxo-3-[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]propyl]amino]-7-[methyl(3-sulfopropyl)amino]-, inner salt (CA INDEX NAME)

PAGE 1-A

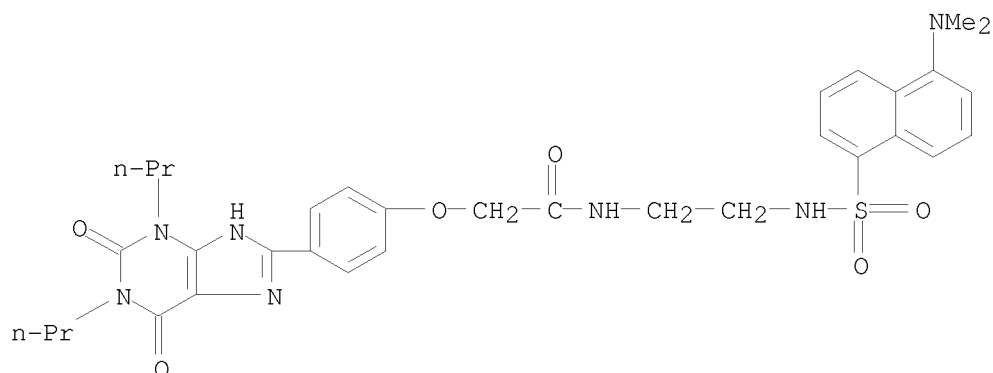


PAGE 1-B



RN 1224605-14-4 CAPLUS
 CN Acetamide, N-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]-

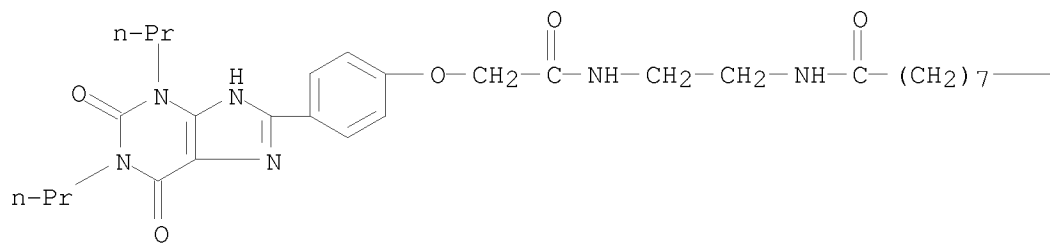
2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]-
(CA INDEX NAME)



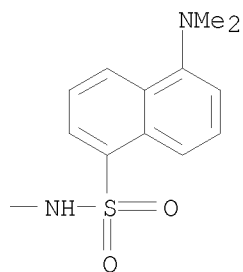
RN 1224605-15-5 CAPLUS

CN Octanamide, 8-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-N-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)

PAGE 1-A



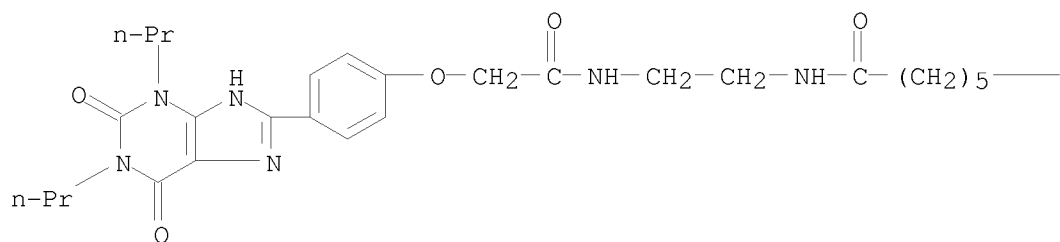
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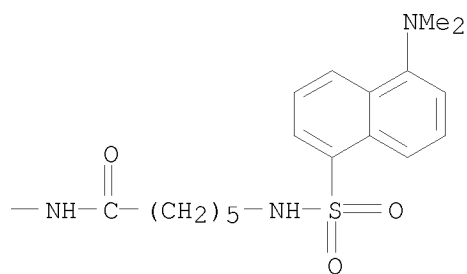
RN 1224605-16-6 CAPLUS

CN Hexanamide, 6-[[[6-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-1-oxohexyl]amino]-N-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)

PAGE 1-A

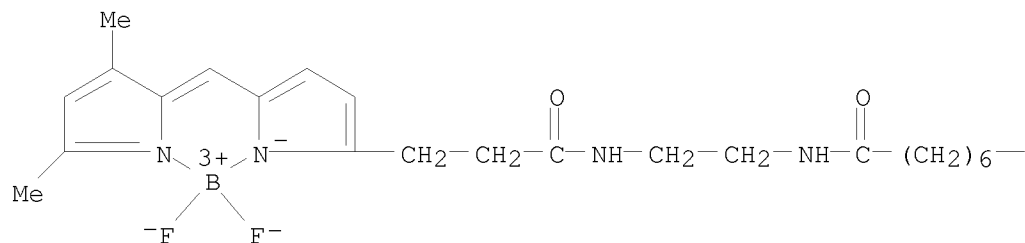


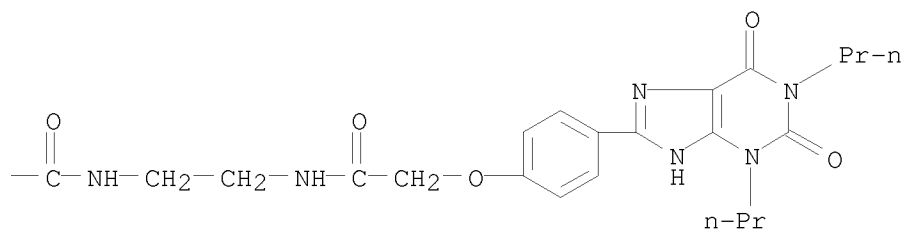
PAGE 1-B



RN 1224699-44-8 CAPLUS
 CN Boron, [N1-[2-[[3-[5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrol-2-yl-κN]-1-oxopropyl]amino]ethyl]-N8-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]octanediamidato]difluoro-, (T-4)- (CA INDEX NAME)

PAGE 1-A



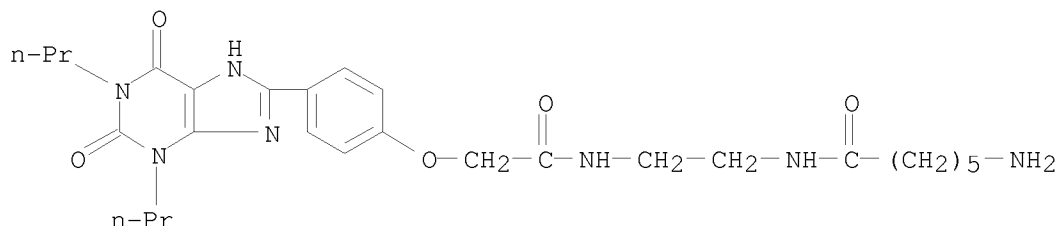


IT 97242-21-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(influence of fluorophore and linker composition on pharmacol. of
fluorescent adenosine A1 receptor ligands)

RN 97242-21-2 CAPLUS

CN Hexanamide, 6-amino-N-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-
1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2007:1472288 CAPLUS

DOCUMENT NUMBER: 148:85762

TITLE: Pharmaceutical combination comprising adenosine A1
receptor antagonists and radiocontrast media for
treatment of radiocontrast media induced nephropathyINVENTOR(S): Hocker, Berthold; Fischer, Yvan; Witte, Klaus;
Ziegler, Dieter

PATENT ASSIGNEE(S): Solvay Pharmaceuticals GmbH, Germany

SOURCE: Eur. Pat. Appl., 19pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

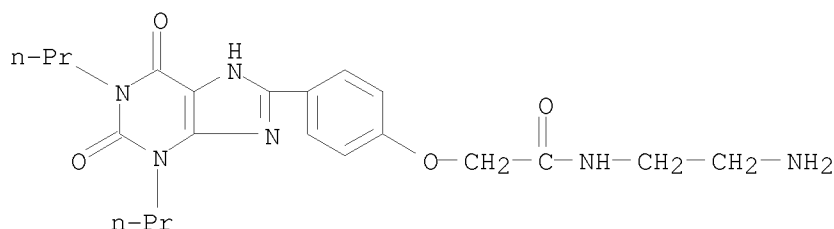
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1870093	A1	20071226	EP 2006-115677	20060619
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				

PRIORITY APPLN. INFO.: EP 2006-115677 20060619

AB The present invention relates to pharmaceutical combinations comprising a
therapeutically effective amount of at least one selective adenosine A1
antagonist combined with at least one radiocontrast media. The invention

also relates to the use of said combinations in the manufacture of a medicament for the treatment of radiocontrast media induced nephropathy. Furthermore, the invention is relating to a kit comprising a single dosage form of said combination of at least one adenosine A1 antagonist and at least one radiocontrast media.

IT 96865-92-8, XAC
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (pharmaceutical combination comprising adenosine A1 receptor
 antagonists and radiocontrast media for treatment of radiocontrast
 media induced nephropathy)
 RN 96865-92-8 CAPLUS
 CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-
 dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
 ACCESSION NUMBER: 2006:301189 CAPLUS
 DOCUMENT NUMBER: 144:343538
 TITLE: Fluorescence-based high content screening of
 compounds for functional response or pharmacological
 properties
 INVENTOR(S): Hill, Steven John; Kellam, Barrie; Briddon, Stephen
 John
 PATENT ASSIGNEE(S): The University of Nottingham, UK
 SOURCE: PCT Int. Appl., 68 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006032926	A2	20060330	WO 2005-GB3709	20050926
WO 2006032926	A9	20060504		
WO 2006032926	A3	20070621		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1792182	A2	20070606	EP 2005-790863	20050926

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
BA, HR, MK, YU

US 20090093001 A1 20090409 US 2008-576035 20081215
PRIORITY APPLN. INFO.: GB 2004-21285 A 20040924
WO 2005-GB3709 W 20050926

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 144:343538

AB A high content screening assay for rapidly screening one or more compds.
to determine functional response or pharmacol. properties thereof, comprises
(i) priming a cell or cell material with a sensor for a biol. response;
(ii) contacting the compound(s) to be tested with the primed cell or cell
material or contacting a cell or cell material which has been contacted
with the compound(s) with the primed cell or cell material; (iii)
simultaneously or subsequently contacting with a fluorescent
agonist or a fluorescent neutral antagonist wherein the binding
of the fluorescent agonist or antagonist and its associated biol.
response are detected or monitored in the same cell and are distinct
allowing sep. readout.

IT 690267-56-2, XAC-BY 630

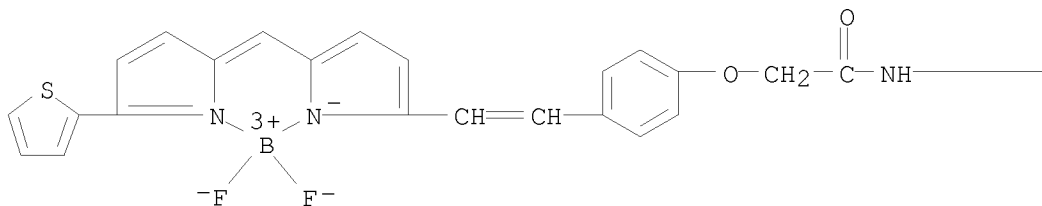
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
(Uses)

(fluorescence-based high content screening of compds. for
functional response or pharmacol. properties)

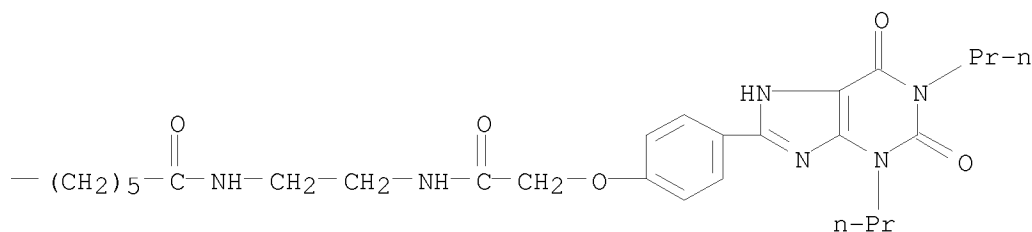
RN 690267-56-2 CAPLUS

CN Boron, difluoro[N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-
purin-8-yl)phenoxy]acetyl]amino]ethyl]-6-[[[4-[(1E)-2-[5-[5-(2-thienyl)-
2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-2-yl-
κN]ethenyl]phenoxy]acetyl]amino]hexanamidato]-, (T-4)- (9CI) (CA
INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

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THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN

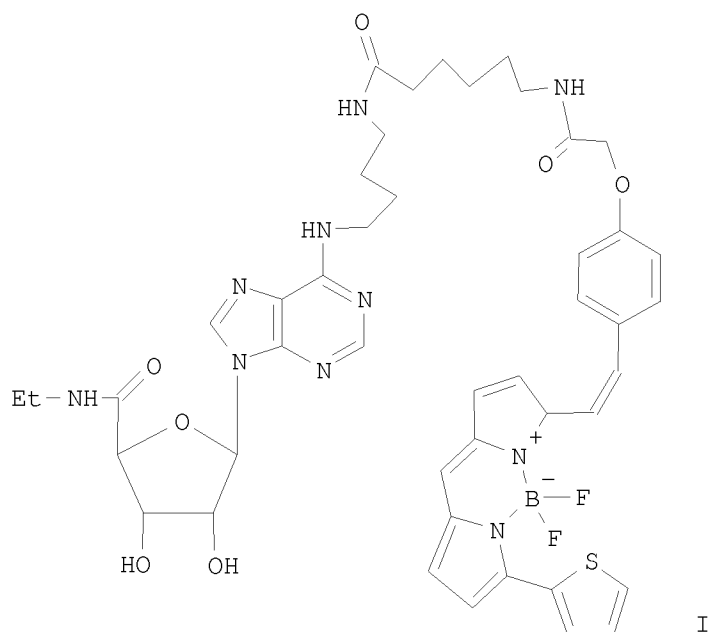
ACCESSION NUMBER: 2004:847667 CAPLUS
DOCUMENT NUMBER: 141:350363
TITLE: Preparation of fluorescently tagged
nucleoside ligands as adenosine A1 receptors
INVENTOR(S): George, Michael; Hill, Stephen John; Kellam, Barrie;
Middleton, Richard John
PATENT ASSIGNEE(S): University of Nottingham, UK
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004088312	A2	20041014	WO 2004-GB1418	20040331
WO 2004088312	A3	20050324		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004225696	A1	20041014	AU 2004-225696	20040331
CA 2521113	A1	20041014	CA 2004-2521113	20040331
EP 1623223	A2	20060208	EP 2004-724650	20040331
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
JP 2006523203	T	20061012	JP 2006-506071	20040331
CN 1860364	A	20061108	CN 2004-80013905	20040331
IN 2005KN01873	A	20061124	IN 2005-KN1873	20050920
US 20060211045	A1	20060921	US 2005-551475	20050930
PRIORITY APPLN. INFO.:			GB 2003-7559	A 20030402
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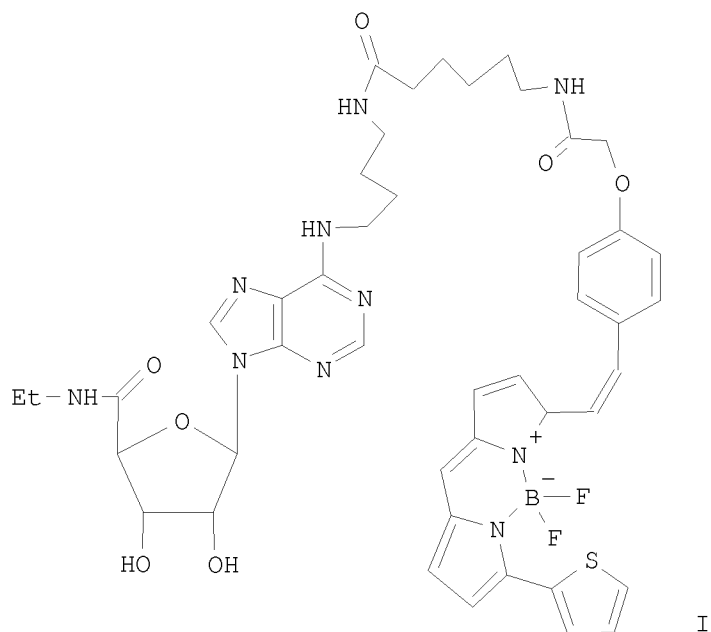
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 141:350363

GI



GI



AB Library comprising a plurality of tagged non-peptide nucleoside ligands (LigJL)mL(JTTag)m(JTL(JLLig)m)p including and salts were prepared, thereof comprising one or a plurality of same or different ligand moieties Lig each linked to a one or a plurality of same or different tag moieties Tag via same or different linker moieties L and same or different linking site or linking functionality JT and JL wherein Lig comprises a GPCR ligand, an

inhibitor of an intracellular enzyme or a substrate or inhibitor of a drug transporter, L is a single bond or heteroatom N, O, S, P, branched or straight chain saturated or unsatd., C1-600 hydrocarbyl; Tag is tagging substrate; m is 1 to 3; p is 0 to 3. G-protein coupled receptor (GPCR) ligand is selected from any compound which is effective as an agonist or antagonist for an adenosine receptor, β adrenoceptor, muscarinic receptor, histamine receptor, an opiate receptor, cannabinoid receptor, chemokine receptor, α adrenoceptor, GABA receptor, prostanoid receptor, 5-HT (serotonin) receptor, an excitatory amino acid receptor (e.g. glutamate), dopamine receptor, protease-activating receptor, neurokinin receptor, angiotensin receptor, oxytocin receptor, leukotriene receptor, nucleotide receptor (purines and pyrimidines), calcium-sensing receptor, TSH receptor, neurotensin receptor, vasopressin receptor, olfactory receptor, nucleobase receptor (e.g. adenosine), lysophosphatidic acid receptor, sphingolipid receptor, tyramine receptor (trace amines), free-fatty acid receptor and cyclic nucleotide receptor; an inhibitor of intracellular enzymes is an inhibitor of cyclic nucleotide phosphodiesterases; and substrate or inhibitor of drug transporter is selected from substrate or inhibitor of an equilibrium based drug transporters or ATP driven pumps such as catecholamine transporter, nucleoside transporter, an ATP-binding cassette transporter, cyclic nucleotide transporter or derivs. or analogs thereof. Thus, I was prepared as adenosine A1 receptor.

IT 690267-56-2P

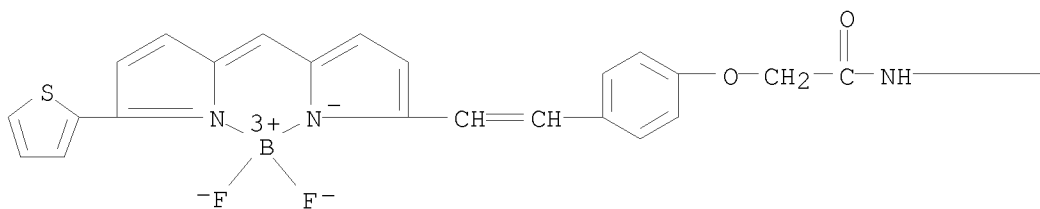
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

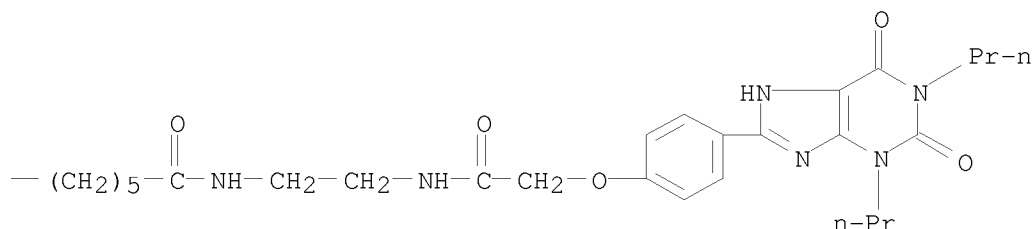
(preparation of fluorescently tagged nucleoside ligands as adenosine receptors)

RN 690267-56-2 CAPLUS

CN Boron, difluoro[N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-6-[[[4-[(1E)-2-[5-[5-(2-thienyl)-2H-pyrrol-2-ylidene- κ N]methyl]-1H-pyrrol-2-yl- κ N]ethenyl]phenoxy]acetyl]amino]hexanamidato]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A





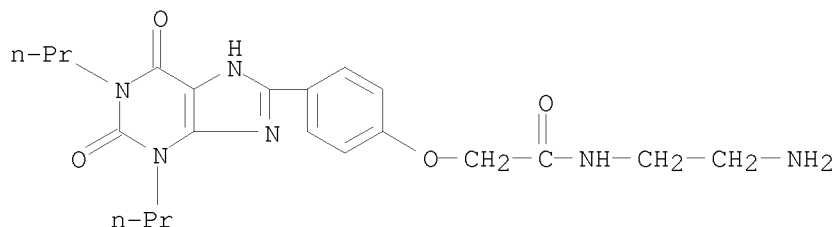
IT 96865-92-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fluorescently tagged nucleoside ligands as adenosine receptors)

RN 96865-92-8 CAPLUS

CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2004:316132 CAPLUS

DOCUMENT NUMBER: 140:418075

TITLE: Quantitative analysis of the formation and diffusion of A1-adenosine receptor-antagonist complexes in single living cells

AUTHOR(S): Briddon, S. J.; Middleton, R. J.; Cordeaux, Y.; Flavin, F. M.; Weinstein, J. A.; George, M. W.; Kellam, B.; Hill, S. J.

CORPORATE SOURCE: Institute of Cell Signalling, Medical School, University of Nottingham, Nottingham, NG7 2UH, UK

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(13), 4673-4678
CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The A1-adenosine receptor (A1-AR) is a G protein-coupled receptor that mediates many of the physiol. effects of adenosine in the brain, heart, kidney, and adipocytes. Currently, ligand interactions with the A1-AR can be quantified on large cell populations only by using radioligand binding. To increase the resolution of these measurements, the authors have designed and characterized a previously undescribed fluorescent antagonist for the A1-AR, XAC-BY630, based on xanthine amine congener (XAC). This compound has been used to quantify ligand-receptor binding at a

single cell level using fluorescence correlation spectroscopy (FCS). XAC-BY630 was a competitive antagonist of A1-AR-mediated inhibition of cAMP accumulation [\log_{10} of the affinity constant ($pK_b = 6.7$)] and stimulation of inositol phosphate accumulation ($pK_b = 6.5$). Specific binding of XAC-BY630 to cell surface A1-AR could also be visualized in living Chinese hamster ovary (CHO)-A1 cells by using confocal microscopy. FCS anal. of XAC-BY630 binding to the membrane of CHO-A1 cells revealed three components with diffusion times (τ_D) of 62 μs (τ_{D1} , free ligand), 17 ms (τ_{D2} , A1-AR-ligand), and 320 ms (τ_{D3}). Confirmation that τ_{D2} resulted from diffusion of ligand-receptor complexes came from the similar diffusion time observed for the fluorescent A1-AR-Topaz fusion protein (15 ms). Quantification of τ_{D2} showed that the number of receptor-ligand complexes increased with increasing free ligand concentration and was decreased by the selective A1-AR antagonist, 8-cyclopentyl-1,3-dipropylxanthine. The combination of FCS with XAC-BY630 will be a powerful tool for the characterization of ligand-A1-AR interactions in single living cells in health and disease.

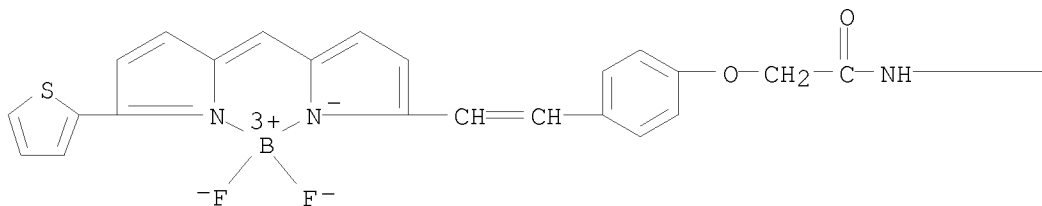
IT 690267-56-2, XAC-BY 630

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses) (design and pharmacol. characterization of fluorescent xanthine amine congener derivative for quant. anal. of formation and diffusion of A1-adenosine receptor-antagonist complexes in single living cells)

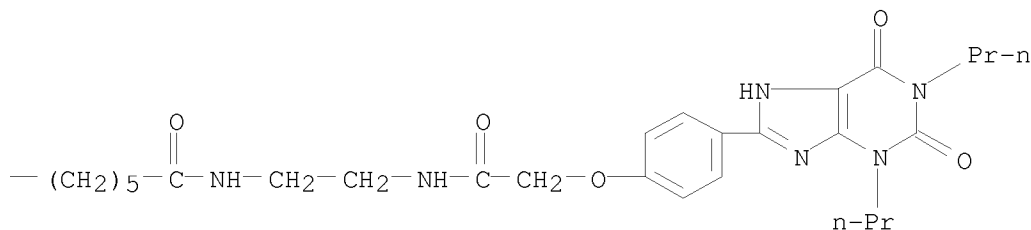
RN 690267-56-2 CAPLUS

CN Boron, difluoro[N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-6-[[[4-[(1E)-2-[5-[5-(2-thienyl)-2H-pyrrol-2-ylidene- κN]methyl]-1H-pyrrol-2-yl]- κN]ethenyl]phenoxy]acetyl]amino]hexanamidato]-, (T-4)- (9CI) (CA INDEX NAME)

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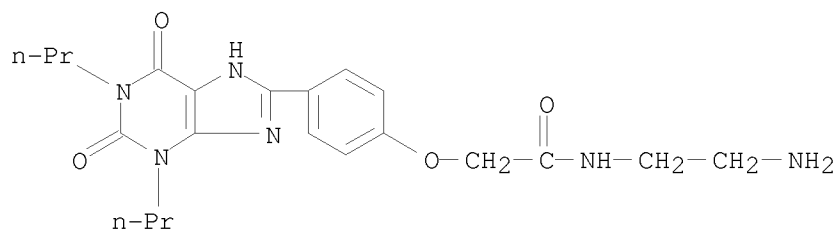
IT 96865-92-8, Xanthine amine congener 690267-56-2D, complexes with A1-adenosine receptor

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(design and pharmacol. characterization of fluorescent xanthine amine congener derivative for quant. anal. of formation and diffusion of A1-adenosine receptor-antagonist complexes in single living cells)

RN 96865-92-8 CAPLUS

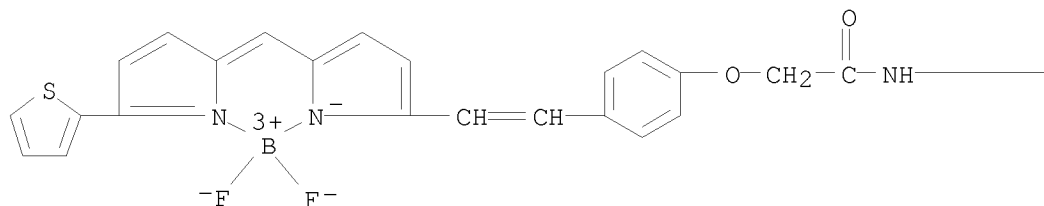
CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



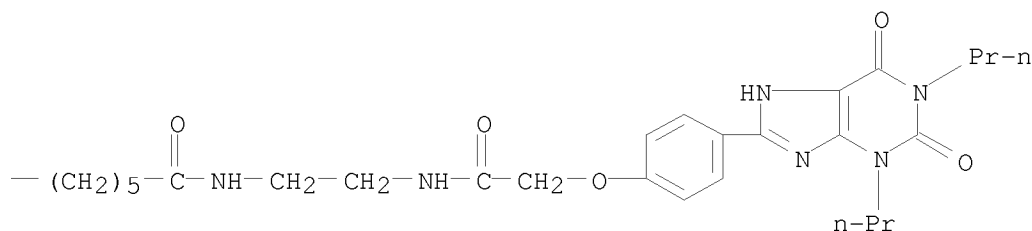
RN 690267-56-2 CAPLUS

CN Boron, difluoro[N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-6-[[[4-[(1E)-2-[5-[5-(2-thienyl)-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-2-yl-κN]ethenyl]phenoxy]acetyl]amino]hexanamidato]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



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OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (42 CITINGS)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1999:405112 CAPLUS
DOCUMENT NUMBER: 131:56155

TITLE: Methods for the simultaneous identification of novel biological targets and lead structures for drug development using combinatorial libraries and probes

INVENTOR(S): Heefner, Donald L.; Zepp, Charles M.; Gao, Yun; Jones, Steven W.

PATENT ASSIGNEE(S): Sepracor Inc., USA

SOURCE: PCT Int. Appl., 125 pp.
CODEN: PIXXD2

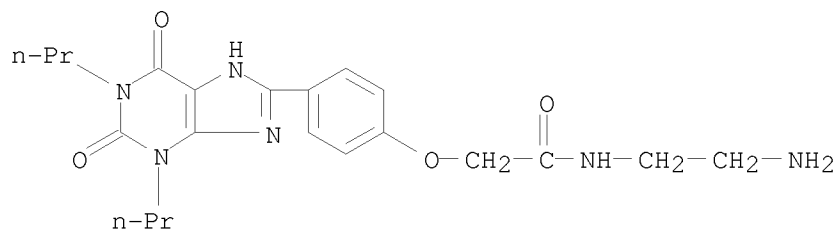
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

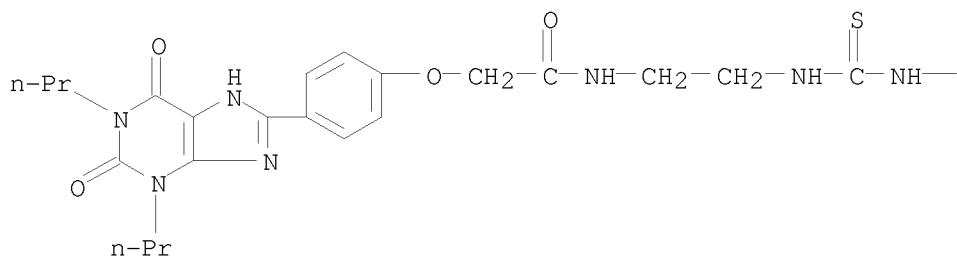
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9931267	A1	19990624	WO 1998-US26894	19981218
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2314422	A1	19990624	CA 1998-2314422	19981218
AU 9919256	A	19990705	AU 1999-19256	19981218
EP 1049796	A1	20001108	EP 1998-964053	19981218
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002508507	T	20020319	JP 2000-539165	19981218
PRIORITY APPLN. INFO.:				
			US 1997-68035P	P 19971218
			WO 1998-US26894	W 19981218
AB	The combinatorial screening assays and detection methods of the present invention encompass highly diversified libraries of compds. which act as fingerprints to allow for the identification of specific mol. differences existing between biol. samples. The combinatorial screening assay and detection methods of the present invention utilize highly diversified libraries of compds. to interrogate and characterize complex mixts. in order to identify specific mol. differences existing between biol. samples, which may serve as targets for diagnosis of development of therapeutics. The invention is base, in part, on the design of sensitive, rapid, homogeneous assay systems that permit the evaluation, interrogation, and characterization of samples using complex, highly diversified libraries of mol. probes. The ability to run the high throughput assays in a homogeneous format increases sensitivity of screening. In addition, the homogeneous format allows the mols. which interact to maintain their native or active conformations. Moreover, the homogeneous assay systems of the invention utilize robust detection systems that do not require separation steps for detection of reaction products. The assays of the invention can be used for diagnostics, drug screening and discovery, target-driven discover, and in the field of proteomics and genomics for the identification of disease markers and drug targets.			
IT	96865-92-8 RL: RCT (Reactant); RACT (Reactant or reagent) (identification of novel biol. targets and lead structures for drug development using combinatorial libraries and probes)			
RN	96865-92-8 CAPLUS			
CN	Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)			



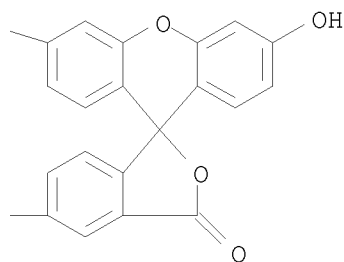
IT 111023-89-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (ligand; identification of novel biol. targets and lead structures for
 drug development using combinatorial libraries and probes)
 RN 111023-89-3 CAPLUS
 CN Acetamide, N-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-
 [9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-
 2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
 (8 CITINGS)
 REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2011 ACS on STN
 ACCESSION NUMBER: 1991:505429 CAPLUS
 DOCUMENT NUMBER: 115:105429
 ORIGINAL REFERENCE NO.: 115:17869a,17872a
 TITLE: Trifunctional agents as a design strategy for
 tailoring ligand properties: irreversible inhibitors

of A1 adenosine receptors

AUTHOR(S): Boring, Daniel L.; Ji, Xiao Duo; Zimmet, Jeff; Taylor, Kirk E.; Stiles, Gary L.; Jacobson, Kenneth A.

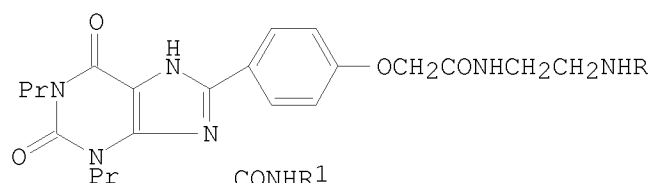
CORPORATE SOURCE: Lab. Bioorg. Chem., Natl. Inst. Diabetes, Dig. Kidney Dis., Bethesda, MD, 20892, USA

SOURCE: Bioconjugate Chemistry (1991), 2(2), 77-88
CODEN: BCCHES; ISSN: 1043-1802

DOCUMENT TYPE: Journal

LANGUAGE: English

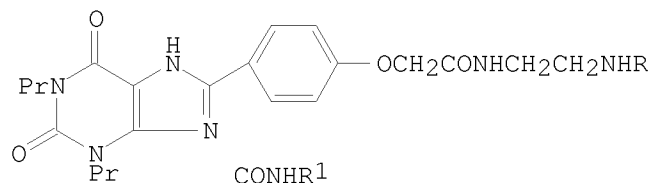
GI



I, R=H

II, R=CSN H

GI



I, R=H

II, R=CSN H

AB The 1,3-phenylene diisothiocyanate conjugate of XAC (I), a potent A1 selective adenosine antagonist) was characterized as an irreversible inhibitor of A1 adenosine receptors. To further extend this work, a series of analogs (e.g., II) were prepared containing a third substituent in the phenylisothiocyanate ring, incorporated to modify the physicochem. or spectroscopic properties of the conjugate. Sym. trifunctional crosslinking reagents bearing two isothiocyanate groups were prepared as general intermediates for crosslinking functionalized congeners and receptors. Xanthine isothiocyanate derivs. containing hydrophilic, fluorescent, or reactive substituents, linked via an amide, thiourea, or methylene group in the 5-position, were synthesized and found to be irreversible inhibitors of A1 adenosine receptors. The effects of the 5-substituent on water solubility and on the A1/A2 selectivity ratios derived from binding assays in rat brain membranes were examined. Inhibition of binding of [3H]-N6-(2-phenylisopropyl)adenosine and [3H]CGS 21680 [2-[2-[4-(2-carboxyethyl)phenyl]ethyl]amino]adenosine-5'-N-

ethylcarboxamide] at central A1 and A2 adenosine receptors, resp., was measured. A conjugate of XAC and 1,3,5-triisothiocyanatobenzene was 894-fold selective for A1 receptors. Reporter groups, such as fluorescent dyes and a spin-label, were included as chain substituents in the irreversibly binding analogs, which were designed for spectroscopic assays, histochem. characterization, and biochem. characterization of the receptor protein.

IT 120059-19-0

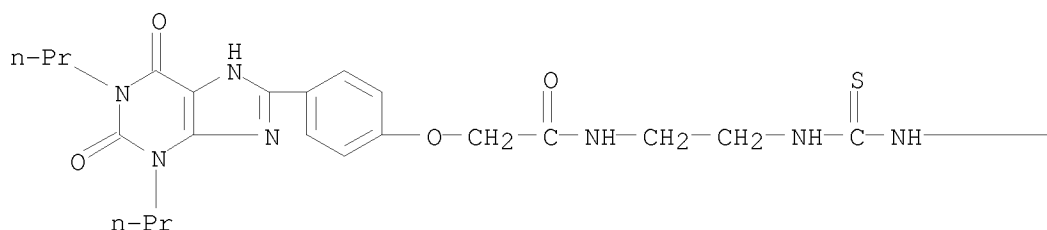
RL: BIOL (Biological study)

(A1 adenosine receptor inhibitory activity of, isothiocyanate derivs. in relation to)

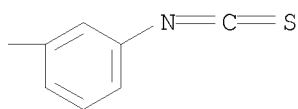
RN 120059-19-0 CAPLUS

CN Acetamide, N-[2-[[[(3-isothiocyanatophenyl)amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]-(CA INDEX NAME)

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IT 133887-95-3P

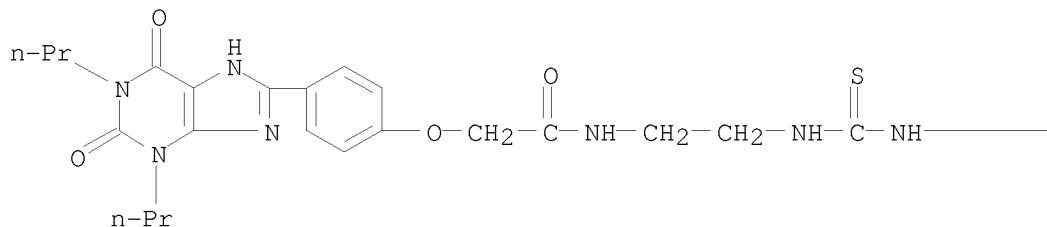
RL: SPN (Synthetic preparation); PREP (Preparation)

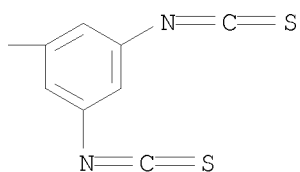
(preparation and A1 adenosine receptor inhibitory activity of)

RN 133887-95-3 CAPLUS

CN Acetamide, N-[2-[[[(3,5-diisothiocyanatophenyl)amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]-(CA INDEX NAME)

PAGE 1-A



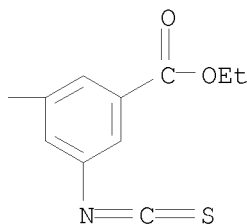
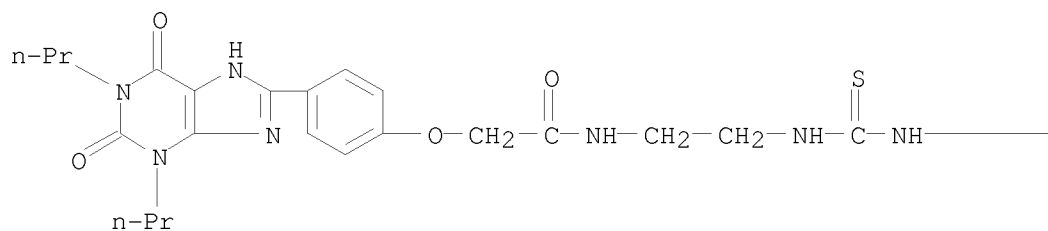


IT 133887-82-8P 133887-99-7P 133888-00-3P
 133888-01-4P 133888-02-5P 133888-03-6P
 133888-04-7P 133888-05-8P 133888-06-9P
 133888-07-0P 133888-08-1P 133888-09-2P
 133888-10-5P 133888-11-6P 133888-12-7P
 133888-13-8P 133888-14-9P 133888-15-0P
 133888-16-1P 133888-17-2P 133888-18-3P
 133909-49-6P 133909-50-9P 133909-51-0P
 133983-35-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and A1 adenosine receptor inhibitory activity of)

RN 133887-82-8 CAPLUS

CN Benzoic acid, 3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]-, ethyl ester (CA INDEX NAME)



RN 133887-99-7 CAPLUS

CN Acetamide, N-[2-[[[(3-aminophenyl)amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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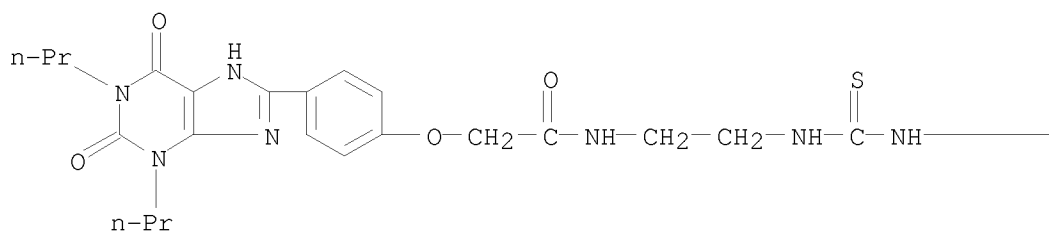
Nc1ccccc1

CN Carbamic acid, [3-[[[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

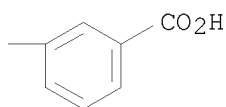
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CN Benzoic acid, 3-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

PAGE 1-A

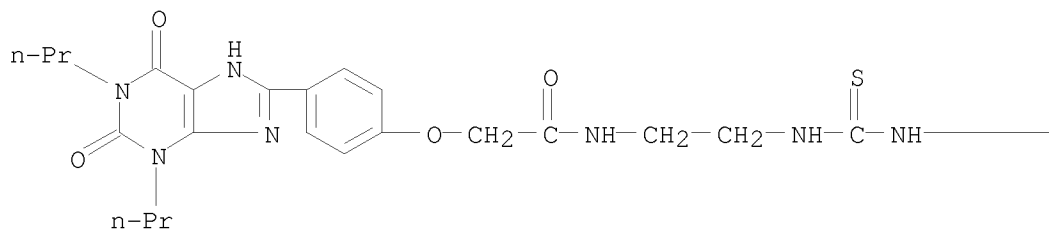


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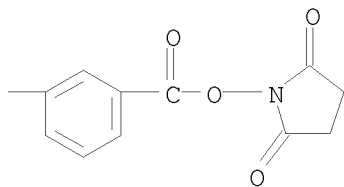


RN 133888-02-5 CAPLUS
CN Benzoic acid, 3-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]-, 2,5-dioxo-1-pyrrolidinyl ester (CA INDEX NAME)

PAGE 1-A

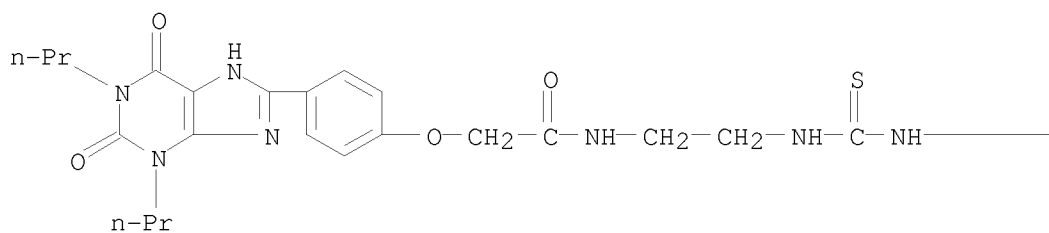


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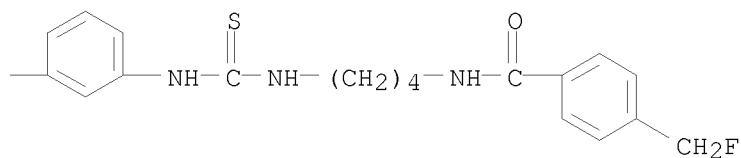


RN 133888-03-6 CAPLUS
CN Benzamide, 4-(fluoromethyl)-N-[4-[[[3-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxomethyl]amino]butyl]- (CA INDEX NAME)

PAGE 1-A

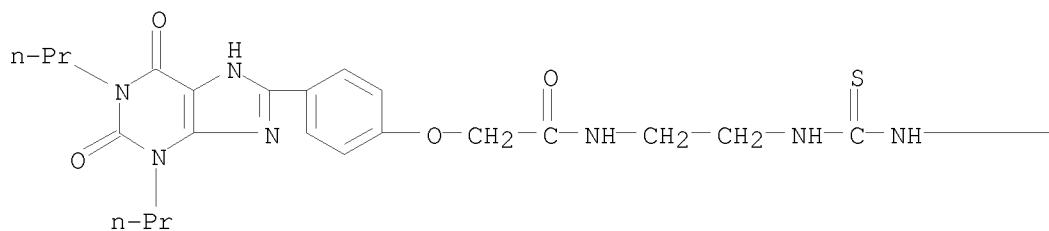


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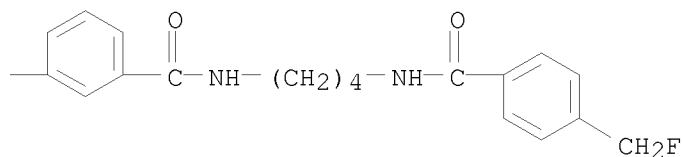


RN 133888-04-7 CAPLUS
 CN Benzamide, N-[4-[[4-(fluoromethyl)benzoyl]amino]butyl]-3-[[[2-[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

PAGE 1-A

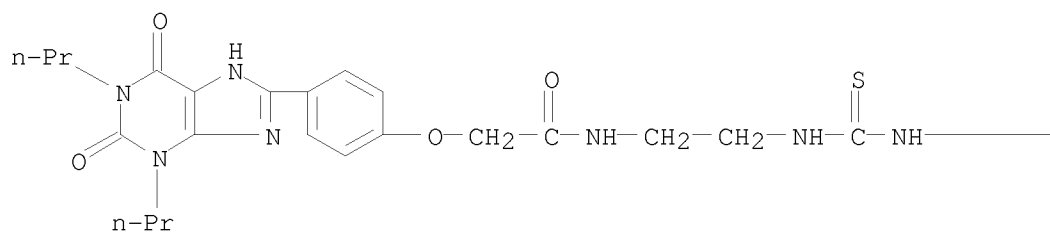


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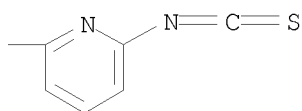


RN 133888-05-8 CAPLUS
 CN Acetamide, N-[2-[[[6-isothiocyanato-2-pyridinyl]amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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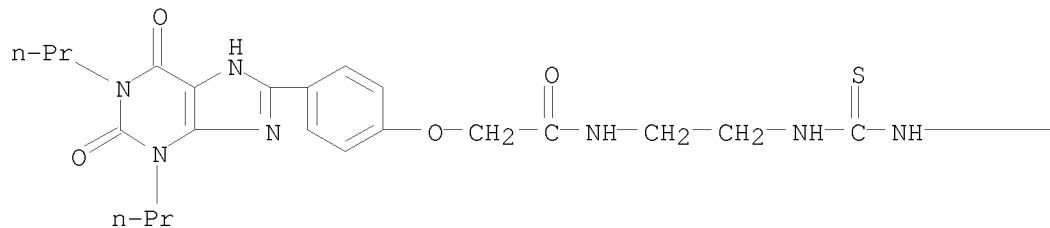


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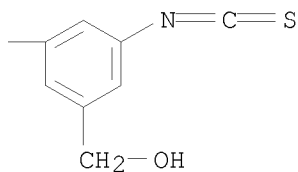


RN 133888-06-9 CAPLUS
 CN Acetamide, N-[2-[[[3-(hydroxymethyl)-5-isothiocyanatophenyl]amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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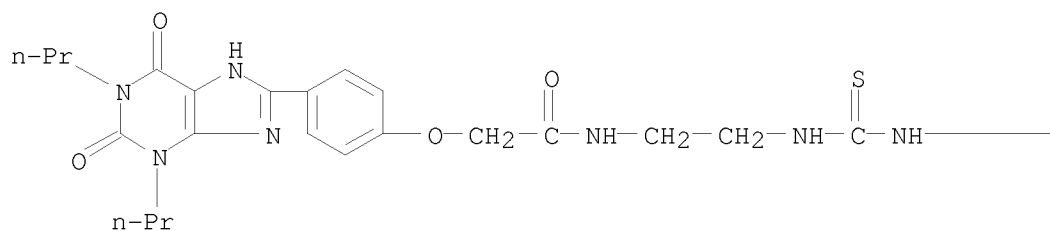


PAGE 1-B



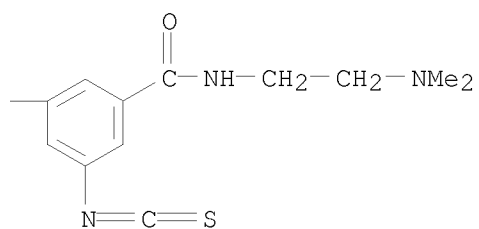
RN 133888-07-0 CAPLUS
 CN Benzamide, N-[2-(dimethylamino)ethyl]-3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]-, hydrochloride (1:1) (CA INDEX NAME)

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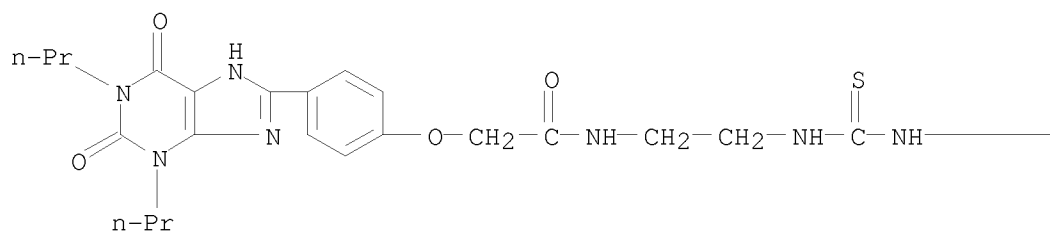
● HCl

PAGE 1-B

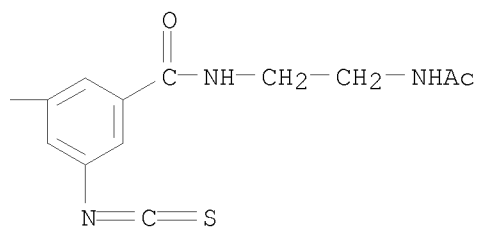


RN 133888-08-1 CAPLUS
 CN Benzamide, N-[2-(acetylamino)ethyl]-3-isothiocyanato-5-[[[2-[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

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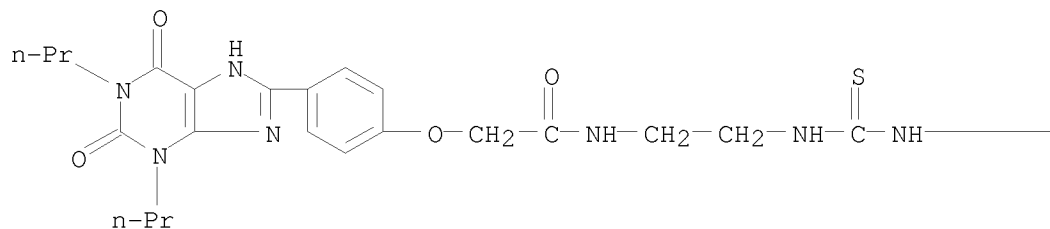
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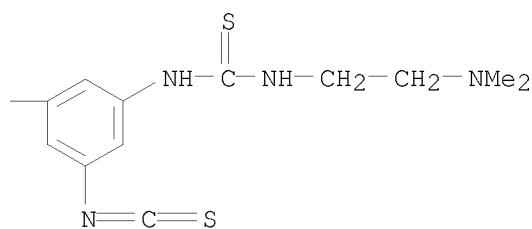
RN 133888-09-2 CAPLUS

CN Acetamide, N-[2-[[[3-[[[2-(dimethylamino)ethyl]amino]thioxomethyl]amino]-5-isothiocyanatophenyl]amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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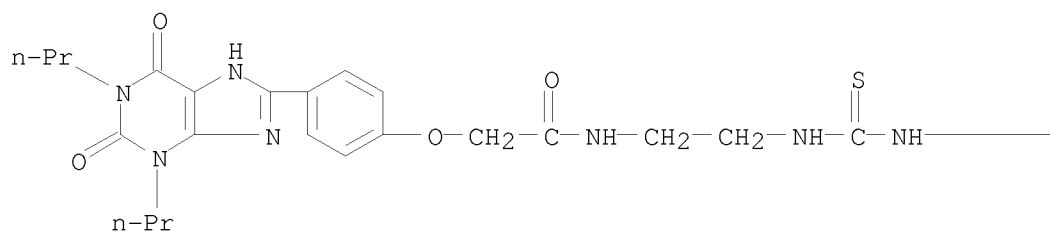
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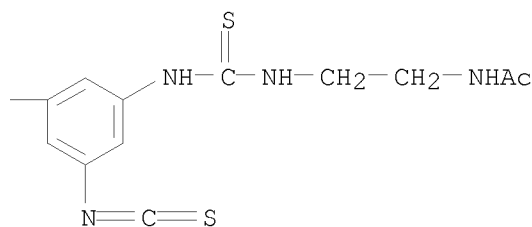
RN 133888-10-5 CAPLUS

CN Acetamide, N-[2-[[[3-[[[2-(acetylamino)ethyl]amino]thioxomethyl]amino]-5-isothiocyanatophenyl]amino]thioxomethyl]amino]ethyl]-2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)

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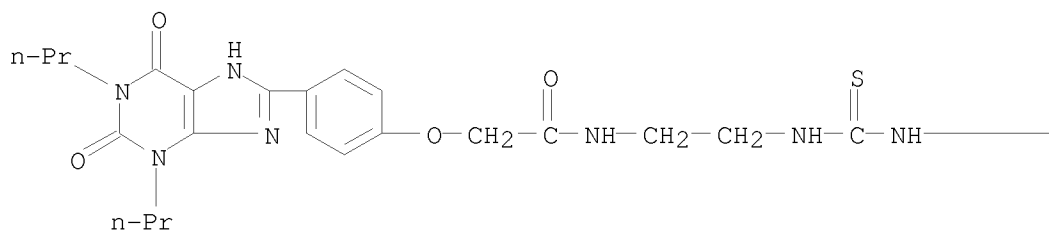
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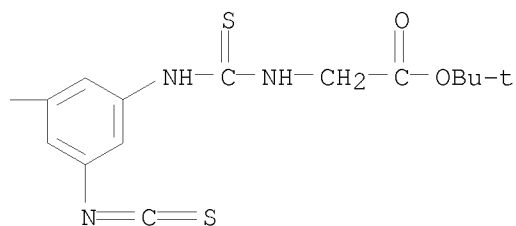
RN 133888-11-6 CAPLUS

CN Glycine, N-[[[3-isothiocyanato-5-[[[[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxomethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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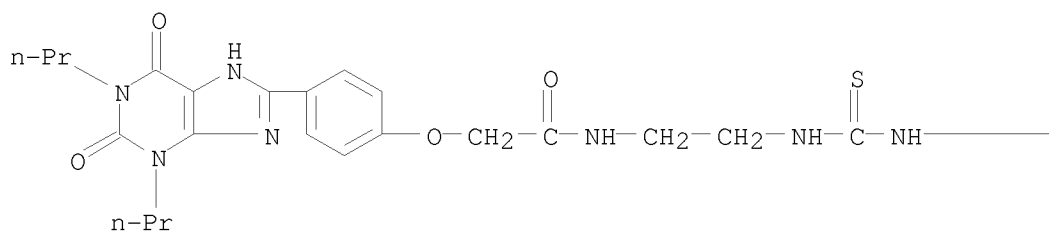
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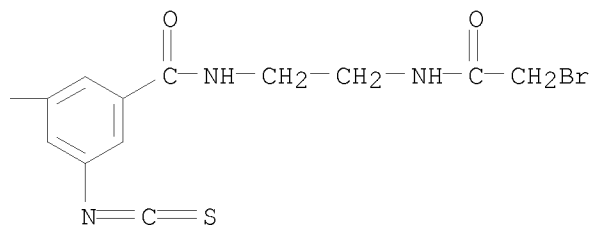
RN 133888-12-7 CAPLUS

CN Benzamide, N-[2-[(2-bromoacetyl)amino]ethyl]-3-isothiocyanato-5-[[[[2-[[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

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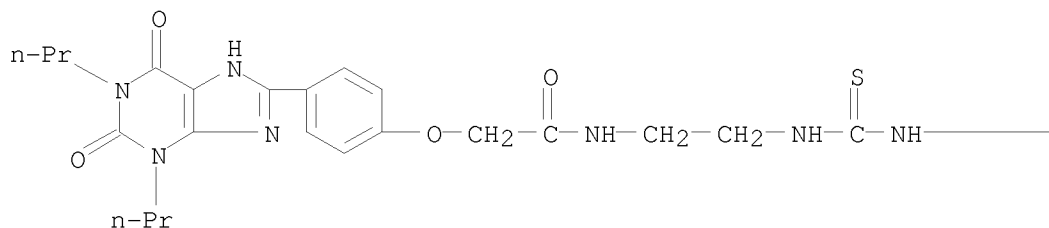
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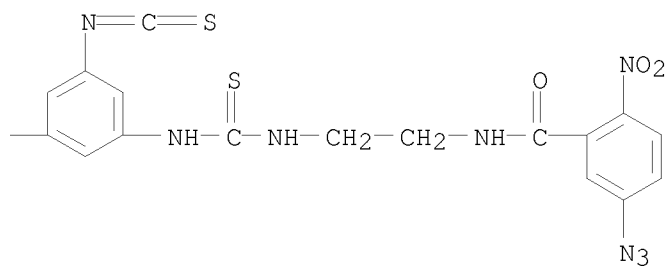
RN 133888-13-8 CAPLUS

CN Benamide, 5-azido-N-[2-[[[3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxomethyl]amino]ethyl]-2-nitro- (CA INDEX NAME)

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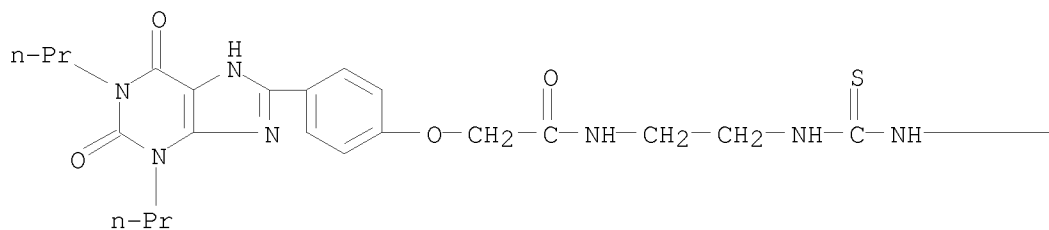
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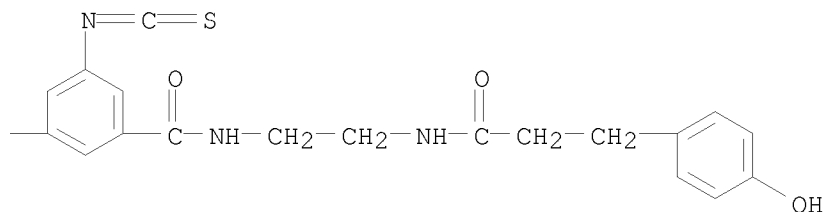
RN 133888-14-9 CAPLUS

CN Benzenepropanamide, 4-hydroxy-N-[2-[[3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]benzoyl]amino]ethyl]- (CA INDEX NAME)

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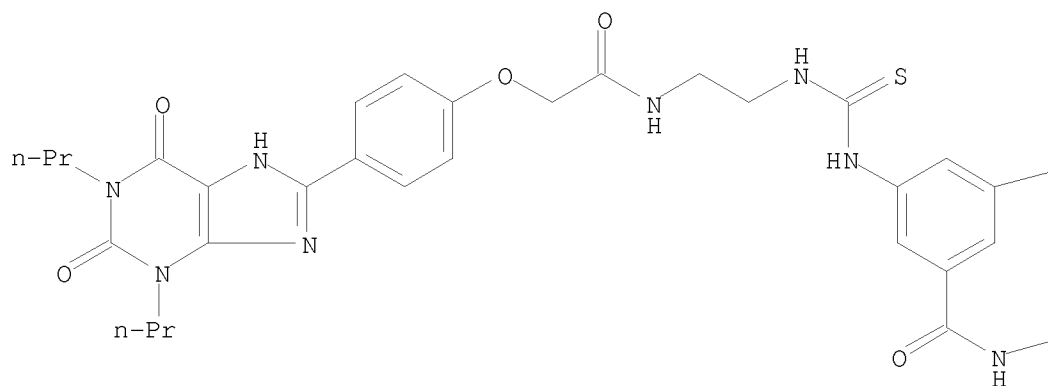
PAGE 1-B



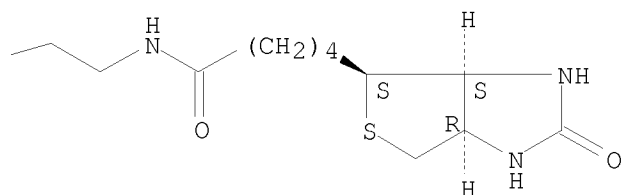
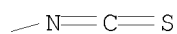
RN 133888-15-0 CAPLUS
 CN 1H-Thieno[3,4-d]imidazole-4-pentanamide,
 hexahydro-N-[2-[[[3-isothiocyanato-5-[[[[2-[[[4-(1,2,3,6-tetrahydro-2,6-
 dioxo-1,3-dipropyl-7H-purin-8-
 yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]benzoyl]amino]ethyl
]-2-oxo-, [3aS-(3aα,4β,6aα)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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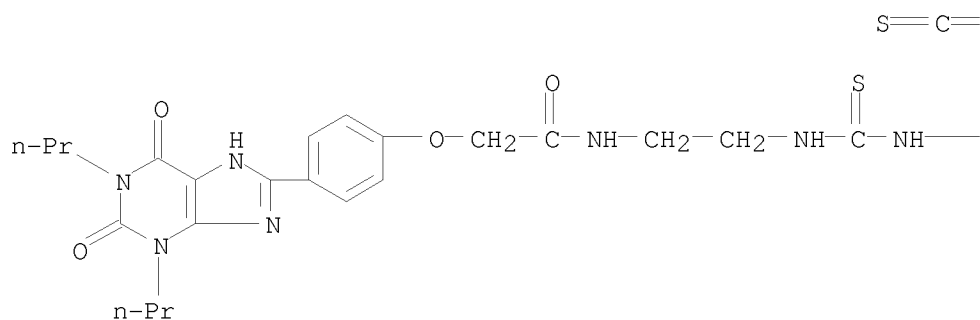


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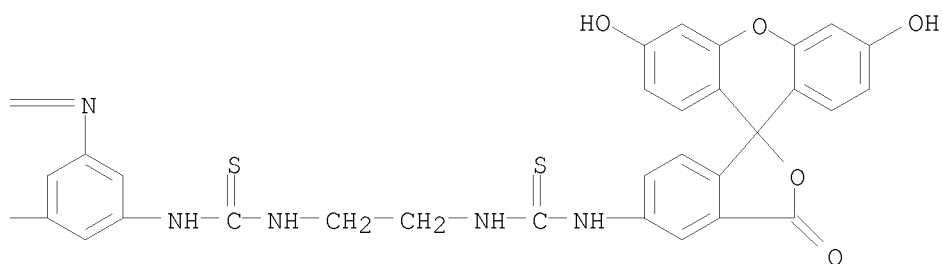


RN 133888-16-1 CAPLUS
 CN Acetamide, N-[2-[[[[[3-[[[[[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-
 1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]amino]thioxometh
 yl]amino]-5-isothiocyanatophenyl]amino]thioxomethyl]amino]ethyl]-2-[4-
 (2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA
 INDEX NAME)

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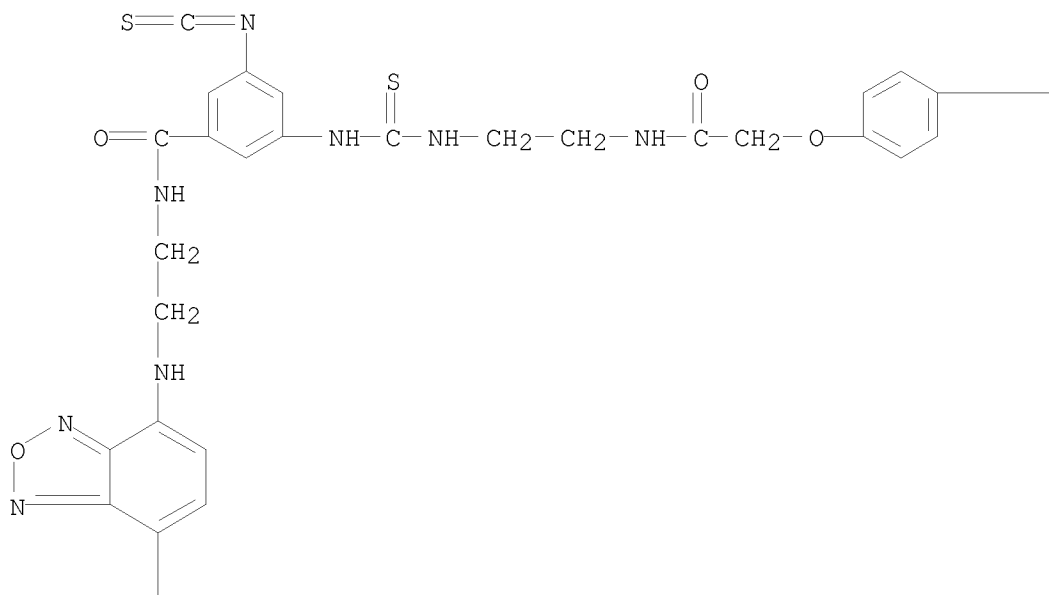
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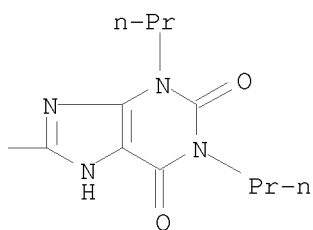
RN 133888-17-2 CAPLUS

CN Benzamide, 3-isothiocyanato-N-[2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethyl]-5-[[[2-[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

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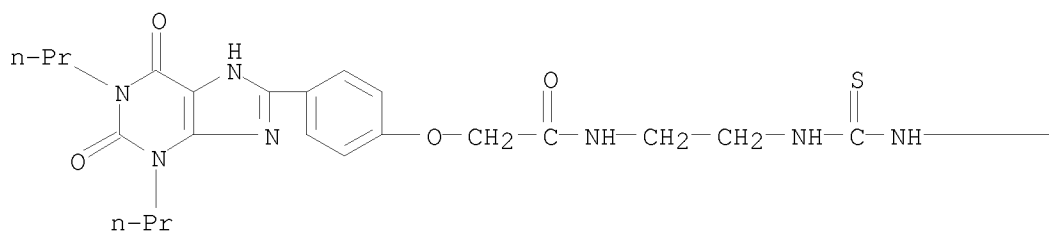


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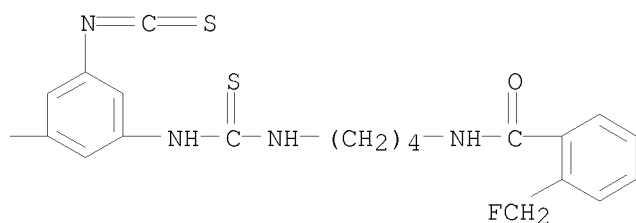


RN 133888-18-3 CAPLUS
 CN Benzamide, 2-(fluoromethyl)-N-[4-[[[3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxomethyl]amino]butyl]- (CA INDEX NAME)

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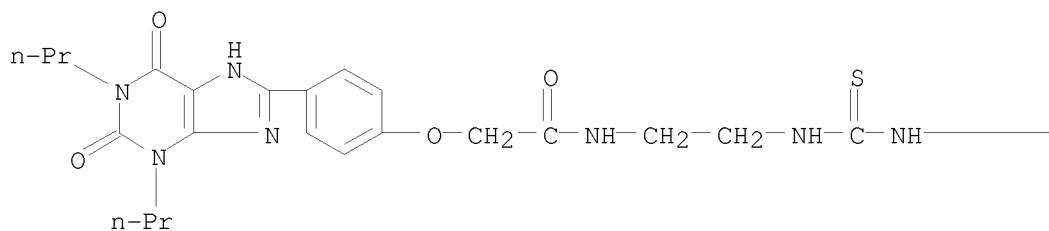


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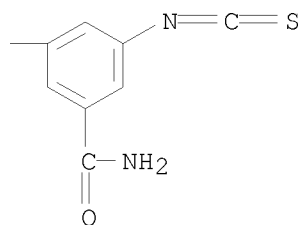


RN 133909-49-6 CAPLUS
 CN Benzamide, 3-isothiocyanato-5-[[[2-[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]- (CA INDEX NAME)

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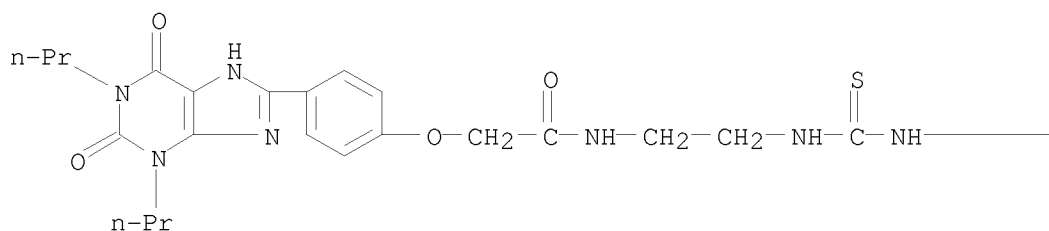


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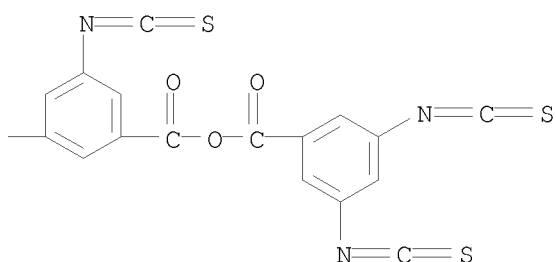


RN 133909-50-9 CAPLUS
 CN Benzoic acid, 3,5-diisothiocyanato-, anhydride with 3-isothiocyanato-5-[[[2-[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]benzoic acid (CA INDEX NAME)

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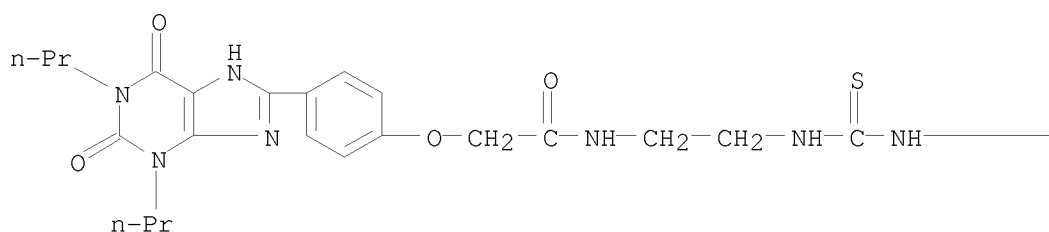


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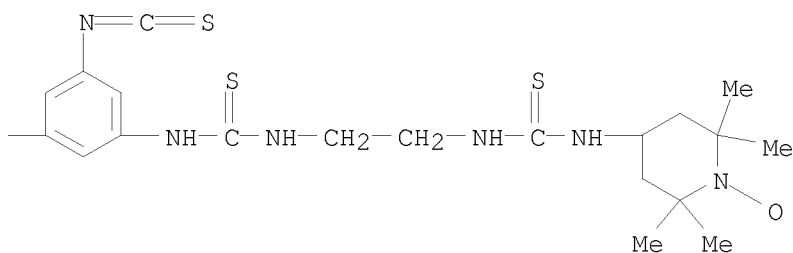


RN 133909-51-0 CAPLUS
 CN 1-Piperidinyloxy, 4-[[[2-[[[3-isothiocyanato-5-[[[2-[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxomethyl]amino]ethyl]amino]thioxomethyl]amino]-2,2,6,6-tetramethyl- (9CI)
 (CA INDEX NAME)

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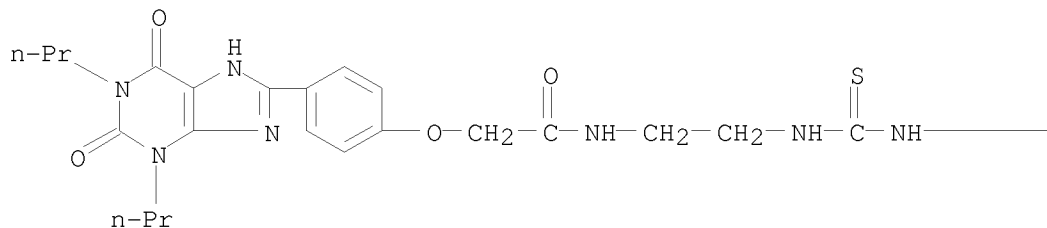
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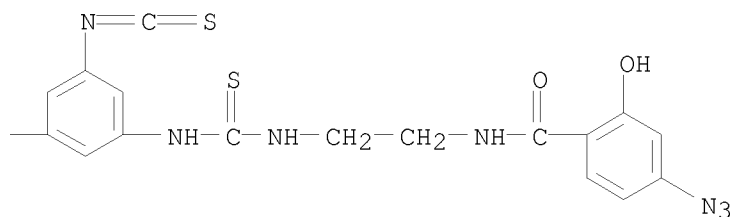
RN 133983-35-4 CAPLUS
 CN Benzamide, 4-azido-2-hydroxy-N-[2-[[[3-isothiocyanato-5-[[[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]thioxomethyl]amino]phenyl]amino]thioxo

methyl]amino]ethyl]- (CA INDEX NAME)

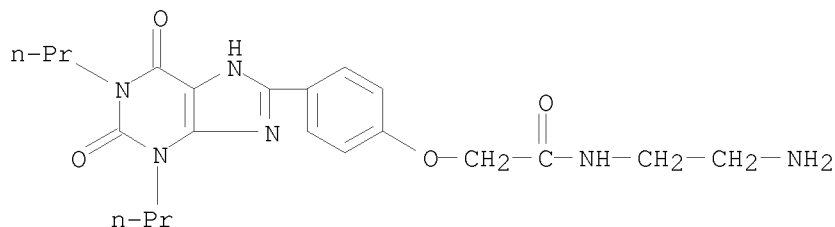
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IT 96865-92-8DP, XAC, phenylene diisocyanate conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as irreversible inhibitors of A1 adenosine receptors)
RN 96865-92-8 CAPLUS
CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

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ACCESSION NUMBER: 1987:611338 CAPLUS

DOCUMENT NUMBER: 107:211338

ORIGINAL REFERENCE NO.: 107:33739a,33742a

TITLE: Molecular probes for extracellular adenosine receptors

AUTHOR(S): Jacobson, Kenneth A.; Ukena, Dieter; Padgett, William;
Kirk, Kenneth L.; Daly, John W.

CORPORATE SOURCE: Lab. Chem., Natl. Inst. Diabetes Dig. Kidney Dis.,
Bethesda, MD, 20892, USA

SOURCE: Biochemical Pharmacology (1987), 36(10), 1697-707
CODEN: BCPA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Derivs. of adenosine receptor agonists (N6-phenyladenosines) and
antagonists (1,3-dialkyl-8-phenylxanthines) bearing functionalized chains

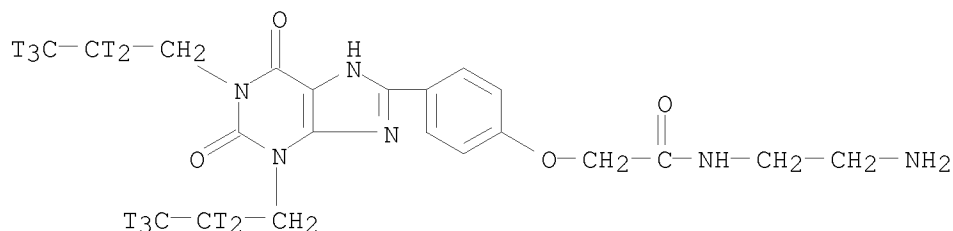
suitable for attachment to other mols. were described. The functionalized congener approach was extended to the synthesis of spectroscopic and other probes for adenosine receptors that retain high affinity (K_2 .apprx. 10^{-9} - 10^{-8} M) in A1-receptor binding. The probes were synthesized from an antagonist xanthine amine congener (XAC), and an adenosine amine congener (ADAC). [3 H]ADAC was synthesized and found to bind highly specifically to A1-adenosine receptors of rat and calf cerebral cortical membranes with K_D values of 1.4 and 0.34 nM resp. The higher affinity in the bovine brain, seen also with many of the probes derived from ADAC and XAC, is associated with Ph substituents. The spectroscopic probes contain a reporter group attached at a distal site of the functionalized chain. These bifunctional ligands may contain a spin label (e.g., the nitroxyl radical 2,2,6,6-tetramethyl-1-piperidinyloxy radical) for ESR, or a fluorescent dye, including fluorescein and 4-nitro-2,1,3-benzoxadiazole, or labels for ^{19}F -NMR spectroscopy. Potential applications of the spectroscopic probes in characterization of adenosine receptors are discussed.

IT 110990-00-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and binding to A1-adenosine receptors)

RN 110990-00-6 CAPLUS

CN Acetamide, N-(2-aminoethyl)-2-[4-[2,3,6,7-tetrahydro-2,6-dioxo-1,3-di(propyl-2,2,3,3,3-t5)-1H-purin-8-yl]phenoxy]- (9CI) (CA INDEX NAME)

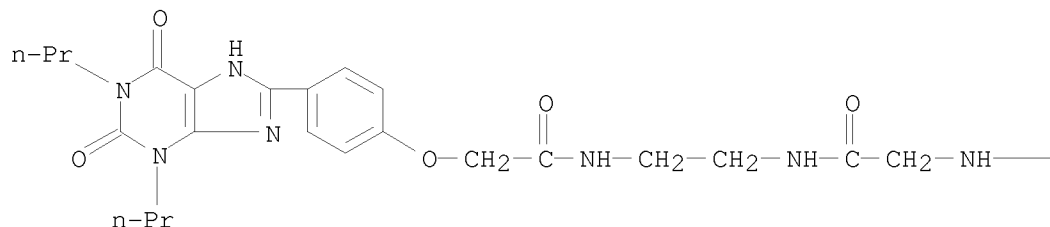


IT 110990-05-1P

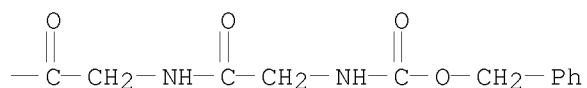
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and deprotection of)

RN 110990-05-1 CAPLUS

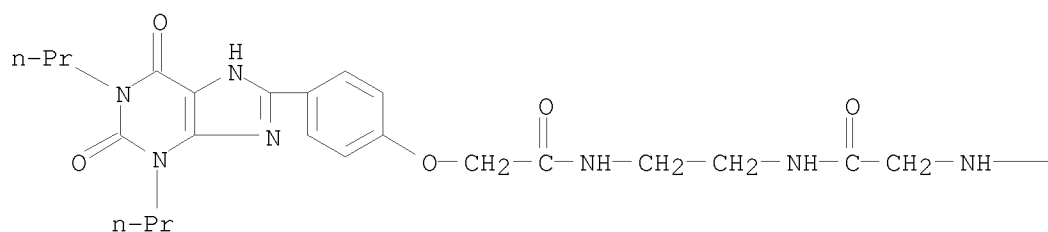
CN Glycinamide, N-[(phenylmethoxy)carbonyl]glycylglycyl-N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)



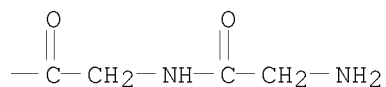
PAGE 1-A



IT 110990-06-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction with fluorescein isothiocyanate or
 biotin derivative)
 RN 110990-06-2 CAPLUS
 CN Glycinamide, glycylglycyl-N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-
 dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-, monohydrobromide
 (9CI) (CA INDEX NAME)

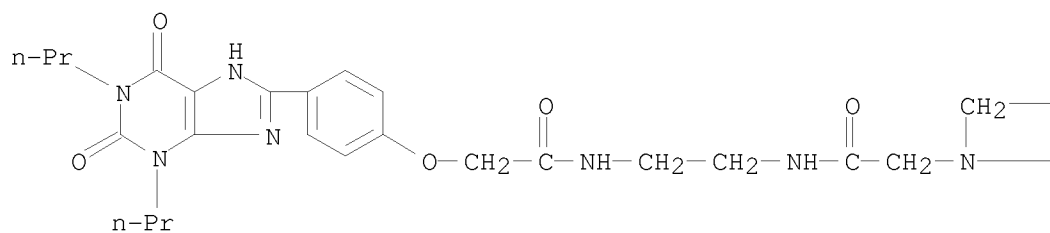


● HBr

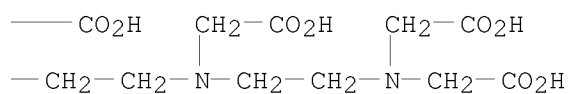


IT 104344-36-7P 110990-01-7P 110990-02-8P
 110990-04-0P 111023-89-3P 111023-91-7P
 111056-21-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as mol. probe for extracellular adenosine receptors)
 RN 104344-36-7 CAPLUS
 CN 3,6,9,12,15-Pentaazaheptadecanoic acid,
 3,6,9-tris(carboxymethyl)-11,16-dioxo-17-[4-(2,3,6,7-tetrahydro-2,6-dioxo-
 1,3-dipropyl-1H-purin-8-yl)phenoxy]- (9CI) (CA INDEX NAME)

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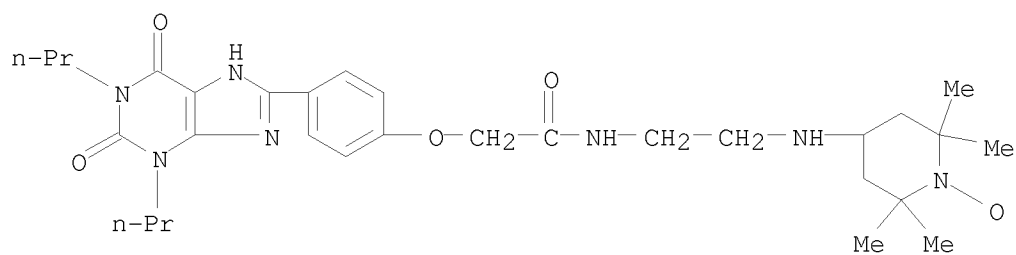


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RN 110990-01-7 CAPLUS

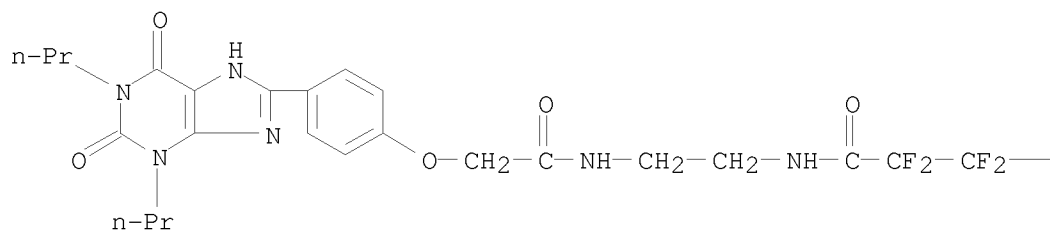
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]amino]- (9CI)
(CA INDEX NAME)



RN 110990-02-8 CAPLUS

CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)

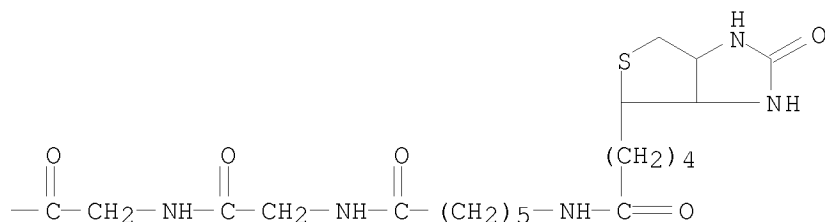
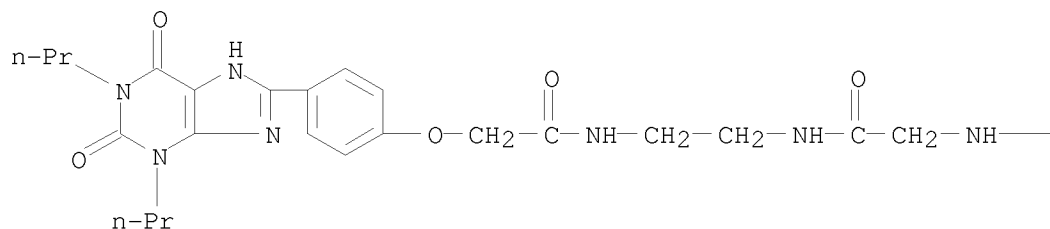
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—CF₃

RN 110990-04-0 CAPLUS

CN Glycinamide, N-[6-[[5-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-1-oxopentyl]amino]-1-oxohexyl]glycylglycyl-N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-, [3aS-(3aα, 4β, 6aα)]- (9CI) (CA INDEX NAME)

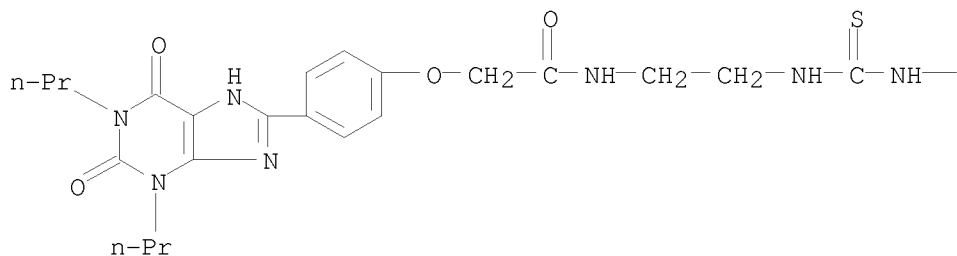


RN 111023-89-3 CAPLUS

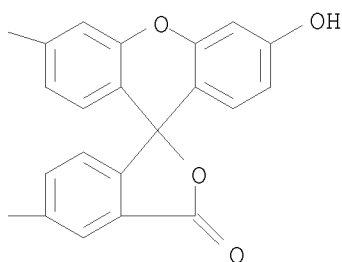
CN Acetamide, N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]-, [3aS-(3aα, 4β, 6aα)]- (CA INDEX NAME)

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HO—

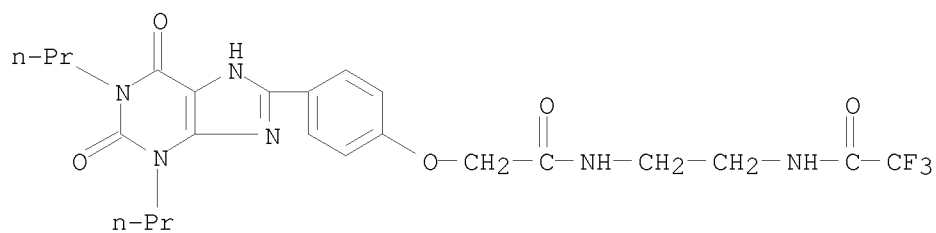


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RN 111023-91-7 CAPLUS

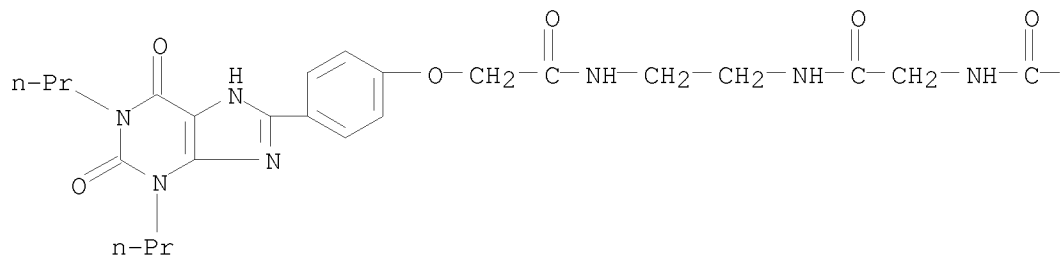
CN Acetamide, 2,2,2-trifluoro-N-[2-[[2-[4-(2,3,6,9-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (CA INDEX NAME)



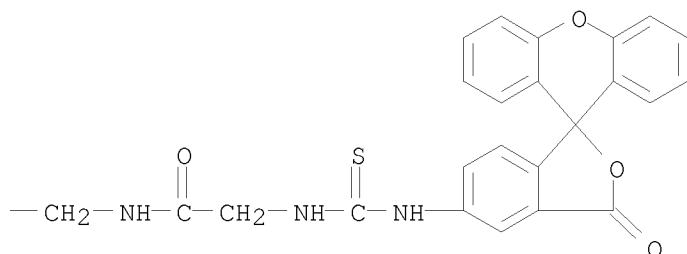
RN 111056-21-4 CAPLUS

CN Glycinamide, N-[[[(3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]glycylglycyl-N-[2-[[[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

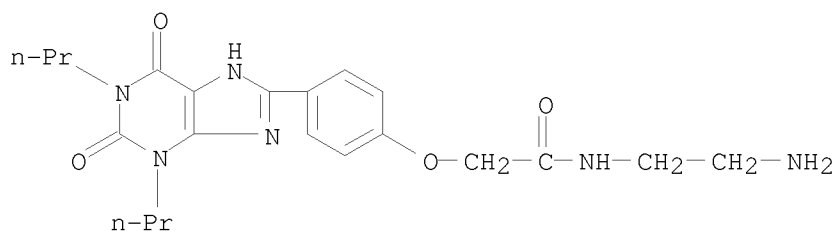
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IT 96865-92-8DP, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as mol. probes for extracellular adenosine receptor)
RN 96865-92-8 CAPLUS
CN Acetamide, N-(2-aminoethyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]- (CA INDEX NAME)



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS
RECORD (13 CITINGS)

=> logoff hold

(FILE 'HOME' ENTERED AT 17:07:03 ON 26 JAN 2011)

FILE 'REGISTRY' ENTERED AT 17:07:21 ON 26 JAN 2011

L1 STRUCTURE UPLOADED

D

L2 13 SEA FILE=REGISTRY SSS SAM L1

L3 284 SEA FILE=REGISTRY SSS FUL L1
L4 254 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L3 AND CAPLUS/LC

FILE 'CAPLUS' ENTERED AT 17:07:56 ON 26 JAN 2011

L5 166 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L4
L6 8 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON L5 AND FLUORES?
D L6 IBIB GI ABS HITSTR 1-8

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	51.08	253.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.96	-6.96

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 17:09:00 ON 26 JAN 2011